Modeling NOx Emissions using the EPA Diesel Emissions Database

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EPA NOx Model

- Agree with the absolute value for diesel fuel property effects on NOx.
- Do not agree with the weighting of specific properties effects on NOx.
  - Small effect of delta cetane on NOx emissions.
  - Does not identify natural cetane number as significant
- Propose re-addressing the draft equation to improve predictive capabilities.

EPA NOx Model

- Coefficient for Cetane Difference term:
  - Does not correlate with past studies,
  - Does not represent the “cetane only” subset of the EPA database accurately.
- Why?
  - More data for Total Aromatics, Specific Gravity and T50 than Cetane Difference.
  - Curvature in Cetane Difference effect not accounted for.
  - Cetane Difference misapplied in many cases (zeros as placeholders).

Definitions

- Cetane Difference - "Difference in cetane number between the test fuel with the cetane improver additive and the base fuel without additive."
- Cetane Difference is undefined (not zero) without knowing the cetane number and emissions of the base fuel and the additized fuel.
  - EPA database incorrectly assigns Cetane Difference values to fuels where the base fuel data is unavailable.

Cetane Difference Effects can be Isolated

- Cetane Difference is the only fuel variable not correlated with other variables.
- Cetane Difference can be changed without affecting any other fuel properties (except nitrogen content).
- The effects of Cetane Difference on emissions can be isolated by examining a subset of the EPA data.

Ethyl Approach

- Take advantage of ability to isolate Cetane Difference effects.
- Apply Cetane Difference as defined:
  - The difference between a base fuel and the same base fuel plus cetane improving additive
- Separate data into 2 groups:
  - Fuels with no Cetane Improver additive.
  - Fuels with Cetane Improver and their corresponding base fuels. This group isolates the effect on emissions of "Cetane Difference."
- Run regression analyses on each group separately.

Advantages

- All data is used as defined.
- Cetane Difference effects are not distorted by larger number of points for Aromatics, Specific Gravity, T50 and other fuel properties.
- More accurately represents Cetane Difference effects.
- Identifies Natural Cetane Number as a significant variable

Emissions from "Base" Fuels

- Analyze all data where Cetane Difference equal to zero.
- Use GLM procedure in SAS. Set Engine ID as a class variable. Manual backward selection.
- NOx <u>not</u> log transformed. Equation form:

$$\boxed{NOx = I + a(TArom) + b(SG) + c(NatCet)}$$

Natural Cetane Number is significant

Emissions from Cetane Improved Fuels

- Equation form:

$$\frac{NOx^{Add} - NOx^{Base}}{NOx^{Base}} = d(CetDif) + e(CetDif^{2})$$
$$+ g((CetDif)(TArom))$$

- Normalizes NOx level for engine, fuel, test cycle, laboratory, etc.
- Squared and crossed terms are significant.

Combined Equation

$$NOx = (I + a(TArom) + b(SG) + c(NatCet)) \quad X$$
$$(d(CetDif) + e(CetDif^{2}) + g(Cetdif)(TArom) + 1))$$

- Allows all data to be used.
- Includes Natural Cetane Number term.
- Shows curvature is significant in Cetane Difference effect.

NOx Estimates

NOx Estimates	**Los Angeles**	**Nationwide**	**% Change**
(Overall Terms)	g/hp-hr	g/hp-hr	
EPA Equation	4.595	4.897	-6.2
Ethyl Equation	4.924	5.243	-6.1

Breakdown of Benefit	EPA	Ethyl
Cetane Difference	16%	26%
Specific Gravity	29%	14%
T50	-2%	0%
Natural Cetane Number	0%	11%
Total Aromatics	57%	49%

Preliminary Analysis

Summary

- Ethyl approach uses all available data.
- Utilizes Cetane Difference appropriately.
- Isolation of Cetane Difference allows a better representation of emissions from cetane improved fuels without sacrificing other fuel property effects.
- Identifies Natural Cetane as significant
- Ethyl recommends the EPA readdress how Cetane Difference is defined and used in modeling emission effects of fuel properties.

Cetane Difference Effect Curvature